Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 58.2

Global applicability domain: Inside

Local applicability domain index: 3.92e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

Image not found
Bis(pentamethylenethiuram)tetrasulfide
Measured: 17.0
Predicted: 21.1

Image not found
Disulfoton
Measured: 219
Predicted: 151

Image not found
Isoamyl ether
Measured: 170
Predicted: 137

Image not found
Isoprothiolane
Measured: 37.2
Predicted: 28.5

Image not found
Phenthoate
Measured: 49.0
Predicted: 17.4